Interface Science - Solutions and Interfaces -

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Visitors

Prof LEVY Ronald M	Rutgers University, USA, 15 October 2001 - 16 October 2001
Prof LEBLANC Roger M	University of Miami, USA, 14 October 2001 - 16 October 2001

Scope of Research

Structure and dynamics of a variety of ionic and nonionic solutions of physical, chemical, and biological interests are systematically studied by NMR under extreme conditions. High pressures and high temperatures are employed to shed light on microscopic controlling factors for the structure and dynamics of solutions. Vibrational spectroscopic studies are carried out to elucidate structure and orientations of organic and water molecules in ultra-thin films. Static and dynamic aspects of membrane-drug and membrane-protein interactions, crystallization of protein monolayers, and advanced dispersion systems are also investigated.

Research Activities (Year 2001)

Presentations

Water and Solutions under Extreme Conditions

NMR and computer simulation studies of structure, dynamics, and reaction of supercritical water, Matubayasi N, 2001 International Association for the Properties of Water and Steam, 9-14 September.

NMR study of aqueous solutions of electrolytes at high temperature and high pressure, Matubayasi N, Nakao N, Kubo M, Tsunashima H, and Nakahara M, High-pressure meeting, 20-22 November.

NMR analysis of hydrothermal decomposition of formic acid: competitive processes into carbon monoxide and water and carbon dioxide and hydrogen, Tsujino Y, Wakai C, Matubayasi N, and Nakahara M, High-pressure meeting, 20-22 November.

Ultra-thin Films

Simultaneous evaluation of refractive-index dispersion and molecular orientation in a ultrathin film by oscillator model simulation and infrared external-reflection spectrometry, Hasegawa T [Kobe Pharm Univ], Umemura J, and Leblanc R M [Univ of Miami], The Pittsburgh Conference, 8 March.

Advanced Dispersion Systems

Surface forces in presence of nano-meter size particles in solution, McNamee C, Matsumoto M, and Nakahara M, 54th Annual Meeting of Division of Colloid and Interface Science, Chem Soc., Jpn, 16 September.

Topics

Water acts as an effective acid at hydrothermal conditions

Water in its neutral form is quantitatively demonstrated at hydrothermal conditions to promote a chemical reaction that proceeds at ambient conditions under the presence of strong acid. By focusing on the dehydration of 1,4-butanediol into tetrahydrofuran, the noncatalytic and acid-catalyzed rate constants are separately determined by varying the hydronium ion concentration. Over a wide range of temperature from moderate to subcritical, neutral water was found to promote the reaction at an effective acid concentration of 10^{-4} -10^{-5} M. Actually, the role of neutral water as an effective acid appears operative even at ambient conditions and becomes manifest at high temperatures. [Fig. 1]

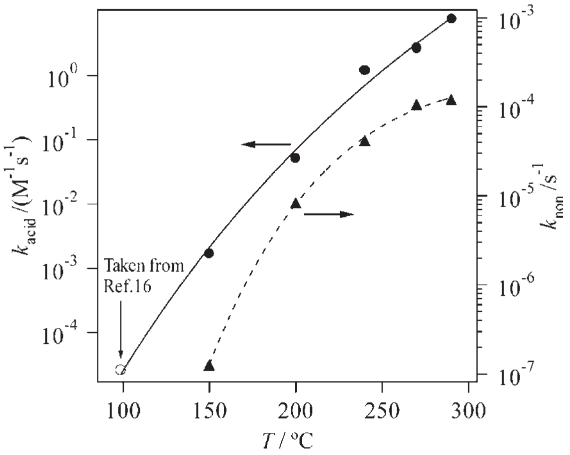

Fig. 1

^{13}C NMR method for determining peptide and protein binding sites in membranes[1]

Reliable NMR criteria for the location and depth of peptides and proteins in membranes were shown by the natural abundance ^{13}C NMR method, which reproduced not only the deep penetration of a channel peptide gramicidin A but also the superficial binding of 18A, a model peptide of apolipoprotein A-I (apoA-I) in plasma. The NMR reliability was ensured by the recent X-ray diffraction data. Our method first provided the atomic-level evidence for native apoA-I binding in egg lecithin (EPC) vesicles (SUV, LUV) and emulsions as model lipoproteins. The result showed not deep but shallow penetration of apoA-I into the membrane interface whose polarity is intermediate between water and the hydrophobic core. [Fig. 2]

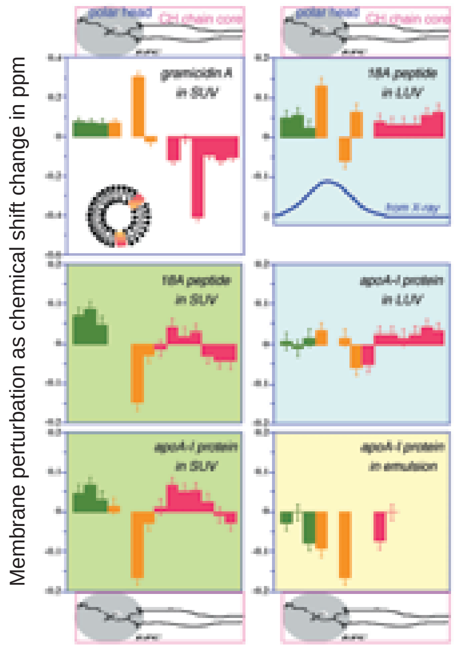

Fig. 2

1. Okamura E et al., *J. Phys. Chem. B*, **105**, 12616-12621 (2001).

Grants

Nakahara M, Collaboratory on Electron Correlations - Toward a New Research Network between Physics and Chemistry, Grant-in-Aid for Creative Scientific Research, 1 April 2001 - 31 March 2006.

Nakahara M, Element Organic Reactions in Super- and Subcritical Water, Grant-in-Aid for Creative Scientific Research (B) (2), 1 April 2001 - 31 March 2003.

Nakahara M, Theoretical and Experimental Studies of Aqueous Solutions under Extreme Conditions, The Japan-USA Joint Research Projects, 1 April 1999 - 31 March 2002.

Umemura J, Study of Spread Monolayers on Liquid Surface by Polarization Modulation Infrared External Spectroscopy, Grants-in-Aid for Scientific Research (B) (2), 1 April 1999 - 31 March 2002.

Hasegawa T and Umemura J, Study of Molecular Recognition Formed in Systematic Molecular Assemblies, The Japan-USA Joint Research Projects, 1 April 2000 - 31 March 2003.

Matubayasi N: Theory of Solutions in the Energy Representation from Ambient to Supercritical, Grant-in-Aid for Scientific Research (C) (2), 1 April 2001 - 31 March 2003.

Awards

Matubayasi N: Helmholtz Award, NMR and computer-simulation studies of supercritical water, International Association for the Properties of Water and Steam, 9 May.

Matubayasi N: Promotion Award, Structure, dynamics, and reactions of supercritical water, Japan society of high-pressure science and technology, 21 November.